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Functional Theory**

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# Quantification of Uncertainties in Nuclear Density Functional Theory

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Reliable predictions of nuclear properties are needed as much to answer fundamental science questions as to use in applications such as reactor physics or data evaluation. Nuclear density functional theory (DFT) is currently the only microscopic, global approach to nuclear structure that is applicable throughout the nuclear chart. In the past few years, considerable effort has been devoted to establishing a general methodology to assess theoretical uncertainties in nuclear DFT calculations. In this paper, we summarize some of the recent progress in this direction. Most of the new material discussed here will be published in separate articles.

## I. INTRODUCTION

The rapid development of leadership-class computing facilities throughout the world, accompanied by targeted programs from funding agencies to foster the use of high-performance computing methods in science, has opened new opportunities in theoretical nuclear structure [1]. Researchers can now address important questions of nuclear science using microscopic approaches rooted in the knowledge of effective nuclear forces and standard methods of quantum mechanics. Recent examples include the explanation of the anomalously long half-life of the  $^{14}\text{C}$  isotope used in carbon dating [2], predictions of neutrino-nucleus currents relevant to physics beyond the standard model [3], and light-ion fusion reactions relevant to the National Ignition Facility [4].

In parallel, there has been an increasing need for accurate and precise data, whether from measurements or simulations, in areas as diverse as nuclear astrophysics [5, 6], reactor physics [7], and data evaluation [8]. In the past, the cost of using standard methods of statistics to estimate theoretical uncertainties in such microscopic approaches was often prohibitive, but this limitation has slowly been disappearing.

Among the few microscopic theories of nuclear structure, density functional theory (DFT) plays a special role, since it is the only one to be applicable across the entire nuclear chart, from the lightest to the heaviest elements. Therefore, DFT is the tool of choice to study phenomena such as nuclear fission [9] or superheavy element predictions [10], but it has also seen applications in tests of

fundamental symmetries [11, 12] and the search for neutrinoless double-beta decay [13].

Here, we present some of the challenges and methodologies used in nuclear DFT to estimate theoretical uncertainties. This topic is covered in greater detail in an invited contribution to a focus issue of the *Journal of Physics G: Nuclear and Particle Physics* on “Enhancing the Interaction between Nuclear Experiment and Theory through Information and Statistics” [14]. In section II, we discuss the main components of nuclear DFT. In section III, we present some of the recent results in uncertainty quantification and error propagation. In section IV, we summarize our conclusions.

## II. NUCLEAR DENSITY FUNCTIONAL THEORY

Density functional theory is a general approach to the quantum many-body system. It is based on a series of theorems by Kohn and Sham, who have shown that theoretically one can find the exact ground-state energy of a system of  $N$  interacting electrons by solving a system of equations characteristic of an independent particle system [15, 16]. This existence result was later extended to the context of nuclear physics [17]. Nuclear DFT is a reformulation of the traditional self-consistent mean-field (SCMF) theory of nuclear structure, which has successfully predicted a broad range of nuclear properties.

The essential component of both the SCMF theory and nuclear DFT is the energy density functional (EDF), which encapsulates all information about the system (in principle). The EDF is a functional of the density of neutrons and protons, as well as of the pairing density [18]. In nuclear DFT, the EDF is treated at the Hartree-Fock-

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Bogoliubov (HFB) approximation level [19]; in the SCMF theory, the EDF is often related to an underlying two-body Hamiltonian, and the HFB approximation may be only the first step of a series of calculations [20]. In any case, the EDF is characterized by a number of coupling constants that are not given by any underlying theory and must therefore be adjusted to some experimental data.

One must emphasize that the Kohn-Sham theorem is only an existence theorem: there is no magic recipe to determine the one EDF that will give the exact energy of the nucleus. In addition, in-medium nuclear forces are poorly known and should in principle be derived from quantum chromodynamics. This situation is in contrast to electronic DFT, where the Coulomb force is known exactly. One should, therefore, consider nuclear DFT and the SCMF theory as inherently imperfect models of the nucleus: this is the first and major source of errors in DFT, which we will refer to as “model errors.” Let us denote by  $\mathbf{x} = (x_1, \dots, x_{n_x})$  the parameters of the EDF (the model). Typically,  $n_x \approx 10 - 20$ . These parameters will be fitted on some  $n_d$  data points  $y_1, \dots, y_{n_d}$ . There could be different types of data: atomic masses, r.m.s. charge radii, mass differences, excitation energies of isomers, and so on. Clearly, given a specific EDF, the choice of the experimental data will impact the overall predictive power of DFT: this is the second source of errors in DFT, which we will label “fitting errors.” A third source of errors, “implementation errors,” is caused by the need to solve the DFT equations numerically. These various sources of uncertainties are discussed in more detail in [14]. Here, we focus only on selected aspects of fitting errors.

### III. QUANTIFYING AND PROPAGATING ERRORS IN NUCLEAR DFT

In discussing uncertainties pertaining to the determination of model parameters, we assume we have an energy density functional that is characterized by the  $n_x$ -vector of unknown parameters  $\mathbf{x}$ . We want to determine the best way to obtain an optimal set of parameters  $\mathbf{x}$  and, at the same time, to quantify the uncertainties associated with this procedure.

Arguably, a very large amount of experimental data exists that potentially could be used to fit the few parameters of an EDF. However, different data types may have different impacts on specific model parameters. For example, researchers using a singular value decomposition analysis pointed out that only a few of the eight parameters of a standard Skyrme EDF are relevant for reproducing nuclear masses [21] or single-particle energies [22]. To constrain every coupling constant of the EDF, therefore, one must introduce different types of data. In practice, the EDF parameters thus are determined by minimizing

the composite  $\chi^2$  function

$$\chi^2(\mathbf{x}) = \frac{1}{n_d - n_x} \sum_{t=1}^{n_T} \sum_{j=1}^{n_t} \left( \frac{y_{tj}(\mathbf{x}) - d_{tj}}{\sigma_t} \right)^2, \quad (1)$$

with  $n_T$  the number of different data types,  $n_t$  the number of data points for type  $t$ , and  $n_d = \sum_t n_t$  the total number of data points over all types. The calculated value of data point number  $j$  of type  $t$  is denoted by  $y_{tj}$ , with  $d_{tj}$  the corresponding experimental value. Because of the different types of data, relative distances must be properly normalized by the quantity  $\sigma_t$ , which represents an estimate of the composite of the modeling and implementation error on data type  $t$ . This strategy was followed in a series of paper by the UNEDF collaboration [23–25].

Minimization of the  $\chi^2$  function yields an “optimal” parametrization of the EDF. One should bear in mind that this notion of optimality depends on, among other things, the choice of the types  $t$  of experimental data, the number of data points for each type  $t$ , and the weight  $\sigma_t$  chosen for each type. In addition, the quality of the optimization is contingent on both the algorithm used and the starting point chosen. Bearing in mind these caveats, one can estimate the covariance matrix by assuming normally distributed errors and local linearity of the model response with respect to variations of model parameters [26]. This approximation has often been used to propagate model errors [27–30].

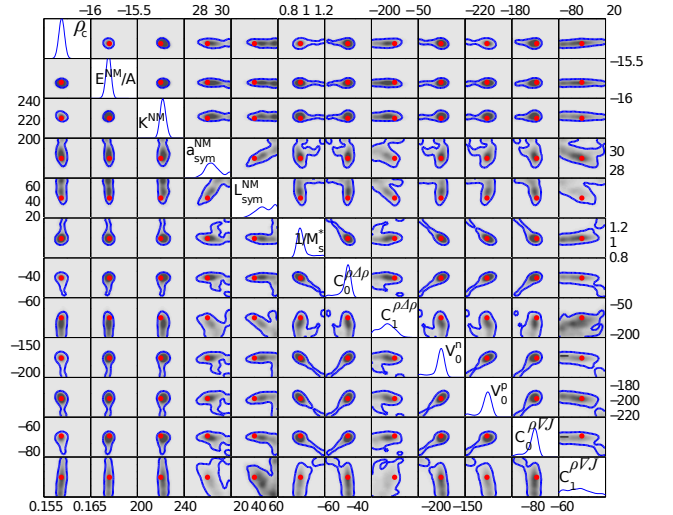


FIG. 1. (Color online) Two- and one-dimensional margins of the 12-d posterior distribution for the UNEDF1 model parameters  $\mathbf{x}$ .

Recently, approaches to uncertainty quantification based on Bayesian statistics have been investigated. In the context of nuclear DFT, such approaches are appealing because they treat model parameters as intrinsically random variables, the true value of which cannot be known with certainty. This perspective is particularly adapted to nuclear structure theory, since the nu-

clear many-problem is unsolvable exactly: only approximations are available (DFT is one of them), and, therefore, uncertainties are unavoidable and should be quantified. We show in figure 1 one of the first examples of a Bayesian posterior distribution corresponding to the UNEDF1  $\chi^2$  function of [25]. The red dots correspond to the UNEDF1 solution itself. Such posterior distributions provide an alternative method for characterizing different sources of uncertainty, and propagating errors in applications [14].

#### IV. CONCLUSIONS

In many important research areas and contemporary applications of nuclear science, nuclear density functional theory represents the only microscopic model of structure and reactions available. Here, we have summarized some of the challenges and recent results in identifying and quantifying theoretical uncertainties inherent to nuclear DFT. In particular, we have emphasized the widespread

use of covariance analysis and the first applications of Bayesian statistics in DFT. With the development of increasingly powerful supercomputers, such methods will most likely gain in popularity and could be applied, for example, to practical applications such as the quantification of errors for fission product yields in neutron-induced fission.

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